LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

LLNL-TR-405901

ParaDyn Implementation in the US Navy's DYSMAS Simulation System: FY08 Progress Report

R. M. Ferencz, A. J. DeGroot, J. I. Lin, E. Zywicz, J. K. Durrenberger, R. J. Sherwood, I. R. Corey

August 1, 2008

Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Contract Information

Contract Number	N00014-08-IP-2-0044
Title of Research	PARADYN implementation into DYSMAS
Principal Investigator	Robert M. Ferencz
Organization	U.S. DOE Lawrence Livermore National Laboratory

Technical Section

Technical Objectives

The goal of this project is to increase the computational efficiency and capacity of the Navy's DYSMAS simulation system for full ship shock response to underwater explosion. Specifically, this project initiates migration to a parallel processing capability for the structural portion of the overall fluid-structure interaction model. The capstone objective for the first phase is to demonstrate operation of the DYSMAS simulation engine with a production model on a Naval Surface Warfare Center (IHD) parallel platform using the ParaDyn code for parallel processing of the structural dynamics.

Technical Approach

The DYSMAS system was created by the Naval Surface Warfare Center (NSWC) and its German Ministry of Defense partners (IABG) by uniting NSWC's GEMINI two-phase flow solver [1] with a modified version of Lawrence Livermore National Laboratory's (LLNL) structural dynamics code DYNA3D [2], designated DYNA_N [3]. Earlier in the present decade the GEMINI code was successfully parallelized, but the DYSMAS structural capability remained serial. Present and future modeling needs clearly indicate that serial processing of the ship structural model is a bottleneck to greater computational throughput and thus greater efficiency and impact of modeling and simulation on ship design and qualification. When seeking a parallel structural dynamics capability to enhance DYSMAS, NSWC-IHD surveyed available options and concluded the least disruptive and most efficient evolution would be to adopt ParaDyn [4], the highly parallel instantiation of DYNA3D created and maintained at LLNL.

This initial demonstration was structured to proceed through several logical gates. The current LLNL version of DYNA3D, which also acts as the finite element technology engine for ParaDyn, was linked to GEMINI using the same communication approach as DYNA_N. This pairing was made operational at NSWC Indian Head Division (IHD) so their engineering personnel could assess the fidelity of DYNA_N and DYNA3D results. The second gate consisted of linking ParaDyn to GEMINI, demonstrating their concurrent operation on an LLNL high-performance cluster, and hosting NSCW-IHD personnel to train them in the LLNL user environment and launch the assessment of computational efficiency. The final gate in this year was the beta release of the 8.1 production version of ParaDyn, which supports coupling to GEMINI, for installation at NSWC-IHD and the continued assessment of the parallel performance of this prototyped coupling.

Progress Statement Summary

This year saw a successful launch to integrate ParaDyn, the high-parallel structural dynamics code from Lawrence Livermore National Laboratory (LLNL), into the DYSMAS system for simulating the response of ship structures to underwater explosion (UNDEX). The current LLNL version of DYNA3D, representing ten years of general development beyond the source branch used to initiate DYNA_N customization for DYSMAS, was first connected to the GEMINI flow code through DYSMAS' Standard Coupler Interface (SCI). This permitted an early 'sanity check' by Naval Surface Warfare Center, Indian Head Division (NSWC-IHD) personnel that equivalent results were generated for their standard UNDEX test problems, thus ensuring the Verification & Validation pedigree they have developed remains intact. The ParaDyn code was then joined to the SCI in a manner requiring no changes to GEMINI. Three NSWC-IHD engineers were twice hosted at LLNL to become familiar with LLNL computer systems, the execution of the prototype software system, and to begin assessment of its accuracy and performance. Scaling data for the flow solver GEMINI was attained up to a one billion cell, 1000 processor run. The NSWC-IHD engineers were granted privileges to continue their evaluations through remote connections to LLNL's Open Computing Facility. Finally, the prototype changes were integrated into the mainline ParaDyn source repository and issued as part of its Version 8.1 beta release. This source was transmitted to NSWC-IHD and in collaboration with LLNL personnel the entire ParaDyn software suite successfully installed and demonstrated on its new SGI Altix machine. The ability of even minor numbers of processors for the structural dynamics to impact overall time-to-solution for DYSMAS has been demonstrated. Assessments of combined parallel efficiencies are beginning to highlight areas for further DYSMAS optimizations.

FY2008 Progress

The first objective in this period was to assess the equivalency of DYNA_N and the current DYNA3D. This was important for two reasons: 1) DYNA3D has evolved for ten years since DYNA_N was derived from a mid-1990s version of its source, and 2) An important motivation for adopting ParaDyn was the intent to maintain a clear connection to the V&V pedigree established for DYSMAS over the past decade. NSWC-IHD shared GEMINI and the DYSMAS Standard Coupler Interface (SCI) definition with LLNL so we could add the appropriate interface calls to the current DYNA3D and retain them in its source repository going forward. This contemporary DYNA3D was verified to operate with GEMINI and then transmitted to NSWC-IHD. Indian Head personnel exercised the GEMINI-DYNA3D simulation on several test problems. Examples such as the “hydrobulge” represented in Figure 1 support their initial assessment that the current DYNA3D is providing results that are in excellent agreement with their baseline tool. We caveat this as an “initial” conclusion because as more complicated problems are examined, subtle differences due to changes in hourglass stabilization or other feature defaults, and even defect remediation, may need to be reconciled.

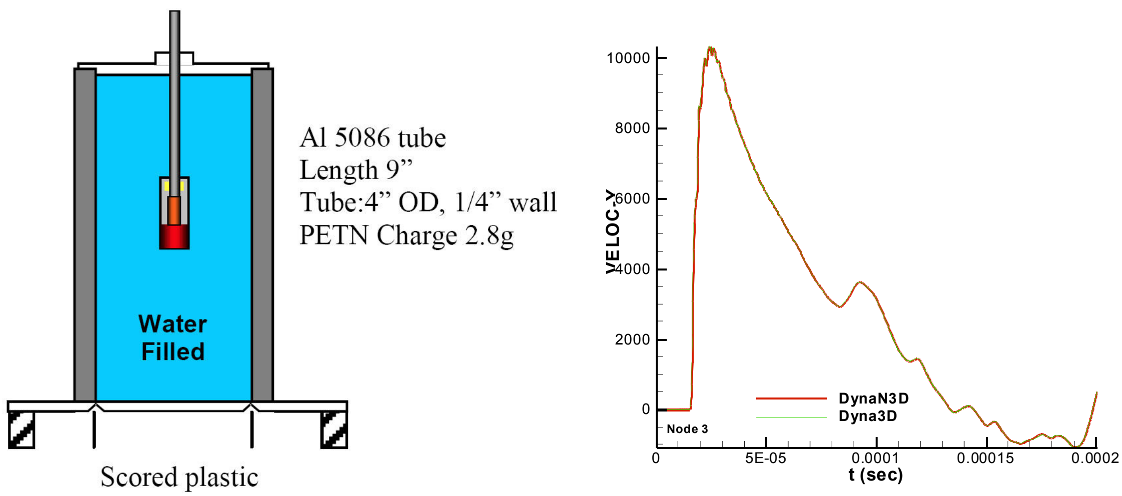

Figure 1. Hydrobulge validation problem used for DYNA3D-to-DYNA_N code verification. The cylinder was represented through an eighth-symmetry model using three continuum elements through the thickness. The time histories show the highly equivalent match of radial velocity at the check location. (Courtesy J.A. Luton, NSWC-IHD.)

As Indian Head personnel engaged in the verification exercise noted above, LLNL personnel embarked on the second objective of creating an initial interface between GEMINI and ParaDyn. The DYSMAS architecture for information flow is illustrated in Figure 2. A single process within GEMINI gathers all nodal forces from the fluid bearing on the structure. These resultants are passed through the Standard Coupler Interface to drive the structural dynamics simulation in DYNA_N. The updated velocities and positions of the structural nodes are then passed back through to GEMINI, where the single process scatters those data to the required processes. This interchange need not occur every time step of the simulation. Given the CFL stability conditions separately limiting time step size in the flow and structural domains, it is sometimes advantageous to permit the structural solver to sub-cycle, i.e., compute several successive smaller time steps, before passing an update to the flow domain.

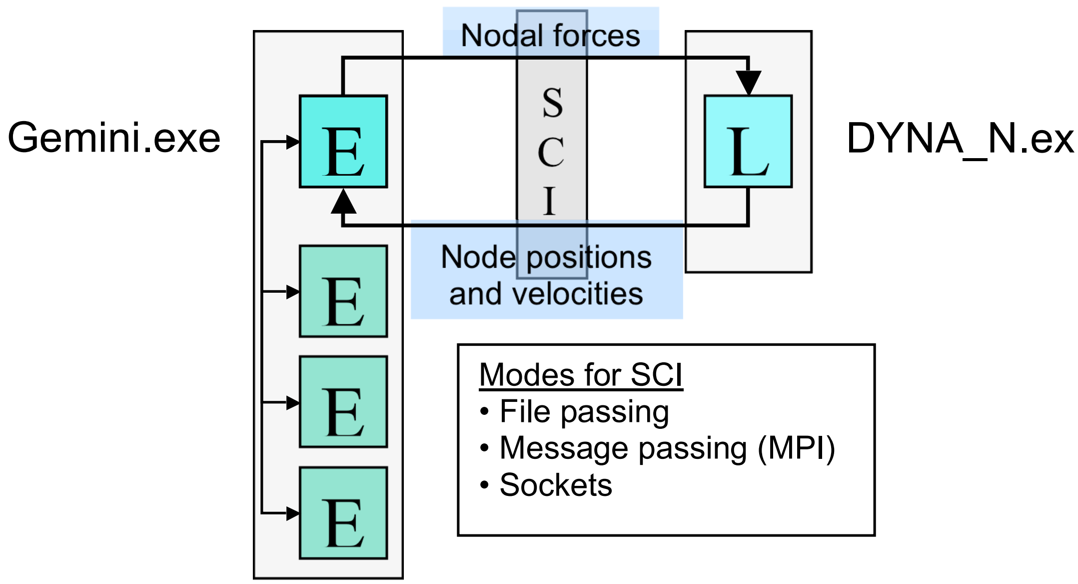

Figure 2. Schematic representation of the DYSMAS Standard Coupler Interface for information exchange between the Eulerian flow code and Lagrangian structural dynamics code. (Courtesy J.A. Luton, NSWC-IHD.)

Given the existing DYSMAS architecture, it was natural for the first-generation integration of ParaDyn to employ a symmetric communication pattern. That is, just as GEMINI uses a 'master' process to gather the nodal forces, use a 'master' process in ParaDyn to receive these forces via the SCI and then scatter them to the subset of ParaDyn processes encompassing all the effected nodes. This communication might be described in shorthand as $m \rightarrow 1 \rightarrow 1 \rightarrow n$ (and its reverse). This approach, while not optimal for performance, had the benefit of confining the immediate changes to ParaDyn alone and thus limiting the scope of possible debugging as initial code issues were resolved.

By mid-December 2007 the initial GEMINI-ParaDyn coupling was operational on one of LLNL's high performance Linux clusters. We were able to host three IHD engineers on site for three days and get one (Luton) activated computer accounts including VPN for subsequent remote access. This visit permitted close interaction between the developers and users and initiated both verification and performance assessment of the prototyped capability. The IHD personnel set up and executed several test problems and visualized the flow domain with an installation of DYSMAS/P. (The structural domain was visualized with the Method Development Group's Griz post-processor.) Some of the scaling data shown later in Figure 4 were measured at that time. This included the opportunity to exercise GEMINI on a greater number of parallel processes than used previously.

Further interaction was supported by an early-April visit by the same IHD team, and at this time we were able to have all three engineers (Luton, Kiddy and Ilamni) use LLNL computer accounts. One model using many triangular shell elements was exercised and a small defect remedied. Communication of element failure flags from the structural domain to GEMINI was verified. Restart capabilities, important for production runs to make effective use of multi-user computational resources, were also confirmed to be operational. Finally, design discussions sketched a potential upgrade path to enhance the parallel communication *within* GEMINI. Testing and characterization activities subsequently continued, facilitated by the VPN accounts issued to all three IHD engineers for remote access to LLNL's Open Computing Facility.

After the first visit, LLNL activities turned to the third objective of having the prototype GEMINI-ParaDyn coupling installed and demonstrated at NSWC-IHD. The target IHD system is an SGI Altix 4700 having 512 cores and sharing 512 GB RAM through a NUMA (Non-Uniform Memory Access) architecture. As LLNL does not possess such a platform, we wanted to minimize the needs for conducting remote debugging. Thus the strategy adopted was to synchronize delivery to NSWC-IHD with release of the 8.1 beta version of ParaDyn [5]. This was accomplished in mid-June and the source code transmitted electronically to Indian Head. LLNL and IHD personnel worked together to compile the necessary components of the ParaDyn Suite: Mili database library, DynPart mesh partitioner, ParaDyn simulation engine, xMiliCS to consolidate partitioned Mili databases, and the Griz visualizer. Efforts focused mainly on issues of coordinating consistent levels of Fortran compiler maintenance patches, third-party library locations, etc.

Figure 3 shows the structural domain for an existing DYSMAS production simulation model. With only 295,000 structural elements, a flow domain of 96 million cells dominates the overall computation. To better judge the efficiency of the current prototype, a coarse flow domain of only 16 million cells was also exercised. Using 15 GEMINI processes and 1 ParaDyn process balanced the wall time for the flow and structural simulations. Tripling the resources to 45 and 3 processes yielded a 1.9X reduction in wall time. This is generally consistent with the GEMINI-only data in Figure 4, where on the Linux cluster its parallel efficiency dips to under 75% for a similar processor count (though a constant million cells per processor). Note that Figure 4 shows the GEMINI-only scaling has a more graceful trend on the Altix.

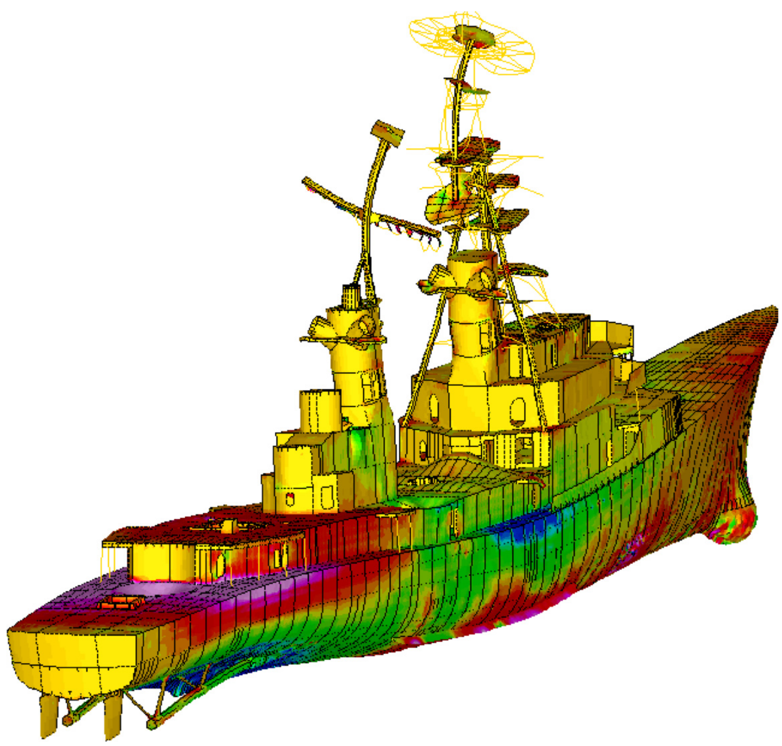

Figure 3. The parallel performance of the GEMINI-ParaDyn coupling was assessed using a 295,000 element structural model of the destroyer Lutjens with flow domain models having 16 and 96 million cells. Deformation under lateral blast magnified for illustrative purposes. (Courtesy J.A. Luton)

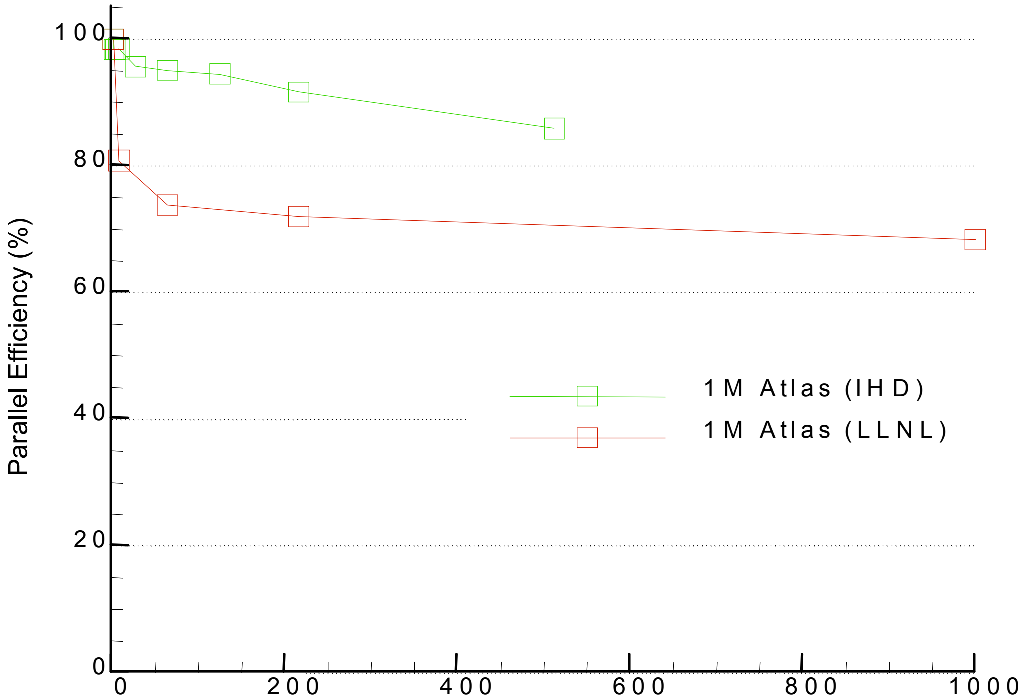

Figure 4. Parallel efficiency measurements for GEMINI assessed using a constant one million cells per processor on an SGI Altix (Atlas IHD) and a Linux cluster with Infiniband interconnect (Atlas LLNL). (Courtesy J.A. Luton)

At this stage the assessment of parallel performance must be considered preliminary. The differing characteristics of the IHD and LLNL machines stress different aspects of code behavior. For large numbers of GEMINI processes some data suggest that greater efficiencies can be realized for the gather of nodal forces to be communicated to the structural domain. This may be realizable through improvement of the existing $m \rightarrow 1 \rightarrow 1 \rightarrow n$ communication pattern and load balance, or may motivate the adoption of a decentralized approach, $m \longleftrightarrow n$, where the necessary fluid and structural subdomains directly exchange the needed data on the relevant parts of the models they host. Or other issues and implementation solutions may be revealed as the investigation proceeds. Nevertheless, the key relevant point after this first year of activity is the impact of parallel execution of the structural model. The software is installed at NSWC-IHD and being exercised in their production environment. As Table 1 illustrates, NSWC-IHD estimates even modest processor counts for ParaDyn will enable order of magnitude speedups on the more detailed structural models that are desired. The initial effort should be judged a success, even as follow-on activities are required. For instance, we cannot claim to have already delivered the next generation DYSMAS, as no effort was made to resolve the output from DYNA3D or ParaDyn to be capability with the post-processor DYSMAS/P. Likewise, specialized features from DYNA_N need to be incorporated into DYNA3D/ParaDyn, including input specifications, to make them available in the parallel setting and assure they migrate forward as a living part of the LLNL source.

Class	Example	dx (cm)	NCells	NElem	Lagrange subcycling	Proc for balanced run	Proc for 2x speedup*	Proc for 10x speedup*
Full ship whipping elastic response	Lutjens shot D	10	96M	295k	5.4	96 / 1	200, 2	1200, 12
Full ship close-in with damage	xCraft	5	26M	380k		32 / 1	64, 2	384, 12
Full ship close-in with damage	Lutjens shot G	10	16M	331k	17	26 / 1	54, 2	312, 12
Full ship shock elastic response	Lutjens shot D (coarse fluid mesh)	25	16M	295k	13.5	16 / 1*	36, 2	200, 12
Full ship shock elastic response	LTA	20	30M	1.1M	6	12 / 1*	24, 2	144, 12
Full ship whipping elastic response	DDG1000	10	96M	5M	20	2 / 1*	4, 2	24, 12

*Estimated

Table 1. Measurements and extrapolations of computational resources required to balance flow and structural simulation wall time and to attain 2X or 10X speedups in time to solution on a Linux cluster with Infiniband interconnect. (Courtesy J.A. Luton.)

References

[1] *GEMINI: The DYSMAS Euler Solver User Manual (Release 4.46),* Naval Surface Warfare Center, Indian Head Division, January 2008.

[2] J. Lin, *DYNA3D: A Nonlinear, Explicit, Three-Dimensional Code for Solid and Structural Mechanics, User Manual (version 6.1),* UCRL-MA-107254, August 2006.

[3] M. Bormann, R. Tewes and R. McKeown, *User's Manual, DYNA_N(3D), A Nonlinear, Explicit, Three-Dimensional Finite Element Code for Solid and Structural Mechanics,* IABGmbH/TA40, NSWCIHD Code 420, May 2001.

[4] C.G. Hoover, A.J. De Groot, and R.J. Sherwood, *ParaDyn: A Parallel Nonlinear, Explicit, Three-Dimensional Code for Solid and Structural Mechanics, User Manual*, Version 7.1, LLNL-SM-400517, December 2007.

[5] A.J. DeGroot, R.J. Sherwood, C.G. Hoover and E.M. Pierce, *ParaDyn Source Code Version 8.1*, Lawrence Livermore National Laboratory, LLNL-CODE-404636, June 2008.